

Quantum effects on the phase diagram of nuclear-like systems

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A Path Integral Monte Carlo method is used to investigate the thermodynamics of nuclear like systems. Systems composed of bosons or fermions interacting via a Lennard-Jones potential with periodic boundary conditions were simulated and the corresponding phase diagrams are constructed. The Path Integral Monte Carlo appears to be a powerful tool for investigating quantum effects in nuclear multifragmentation phenomena.

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Highly excited nuclear systems are good “laboratories” for thermodynamical studies. Due to the van der Waals type of the nucleon-nucleon interaction these systems are supposed [1] to exhibit liquid-gas phase transitions. The connection is however not straight forward due to their small number of constituents, the presence of the Coulomb force and quantum effects. The effect of the Coulomb interaction on the nuclear liquid-gas phase transitions was previously studied (see e.g. Refs. [2, 3]). The effects of other multifragmentation specific features such as finite size (for attempts to describe the finite size effects of the system within Hartree-Fock theories see Refs. [4, 5]) and degree of homogeneity were addressed in Refs. [6–9]. Nuclear multifragmentation of excited nuclear systems was treated with cluster-type models like SMM, MMMC, and MMM [10–12]. In this kind of models a fragmentation event is approached by various size excited nuclear fragments interacting only via their Coulomb field. This approach works very well at small densities where, the average distance between fragments is large enough and fragments don’t interact via nuclear forces. At larger densities, fragments are no longer spherical and the nuclear interaction between them is quite important. At such densities, quantum and shape degeneracy effects play an important role. Indeed, it was proven that a cluster-type statistical multifragmentation model cannot accurately describe the dense branch of the phase diagram [2].

Monte Carlo simulations with classical Lennard-Jones fluids showed that the accurate treatment of fragments’ shape degeneracy leads to the restoration of the Guggenheim shape of the phase diagram [7, 18]. However, the systems considered there were classical. What about quantum ones? This question is addressed in the present paper.

In the present work we perform a simulation of a quantum fluid interacting via a Lennard Jones 6-12 (LJ) fluid. Such simulations are tractable with Path Integral Monte Carlo (PIMC) methods and have been extensively used in solid-state physics (see eg. [13]). The PIMC method is based on the isomorphism that one can achieve between the average value $\langle O \rangle$ of an observable (O) of a N -particle

quantum system and the average value of the the same observable corresponding to a classical N -polymer system. This correspondence was firstly pointed by Feynman in 1972 [14]. Let us briefly present some Path Integral theory. The average value of a system observable, O , writes:

$$\langle O \rangle = \frac{1}{Z} \sum_i e^{-\beta E_i} \langle \Phi_i | O | \Phi_i \rangle \quad (1)$$

where $Z = \sum_i e^{-\beta E_i}$ is the canonical partition function Φ_i is the i th particle wave-function. In a position-space representation, the density matrix writes:

$$\rho(\mathbf{R}, \mathbf{R}'; \beta) = \langle \mathbf{R} | e^{-\beta E} | \mathbf{R}' \rangle = \sum_i e^{-\beta E_i} \Phi_i^* \Phi_i \quad (2)$$

where $\mathbf{R} = \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\}$. So:

$$\langle O \rangle = \frac{1}{Z} \int d\mathbf{R} d\mathbf{R}' \rho(\mathbf{R}, \mathbf{R}'; \beta) \langle \mathbf{R} | O | \mathbf{R}' \rangle \quad (3)$$

For a free particle in a D -dimensional box of size L with periodic boundary conditions (PBC), one has:

$$\Phi_n = \frac{1}{L^{D/2}} e^{-i\mathbf{k}_n \mathbf{r}}. \quad (4)$$

Hence:

$$\begin{aligned} \rho(\mathbf{r}, \mathbf{r}'; \beta) &= \frac{1}{L^D} \sum_n \exp \left[-\beta \lambda \mathbf{k}_n^2 + i\mathbf{k}_n (\mathbf{r} - \mathbf{r}') \right] \\ &= (4\pi\lambda\beta)^{-D/2} \exp \left[\frac{(\mathbf{r} - \mathbf{r}')^2}{4\lambda\beta} \right], \text{ if } \lambda\beta \ll L^2 \end{aligned} \quad (5)$$

where for a particle of mass m , $\lambda = \hbar^2/2m$. The underlying principle of introducing path integrals in *imaginary time* is the product property of the density matrix stating that the low temperature density matrix can be expressed as a product of high-temperature density matrices:

$$e^{-\beta \mathcal{H}} = (e^{-\tau \mathcal{H}})^M \quad (6)$$

where the “time step” $\tau = \beta/M$. Usually the hamiltonian \mathcal{H} is a sum of a kinetic part and a potential one:

$\mathcal{H} = \mathcal{K} + \mathcal{V}$. For very small values of τ one can use the so-called *primitive approximation* [15]:

$$e^{-\tau\mathcal{H}} = e^{-\tau\mathcal{K}} e^{-\tau\mathcal{V}} \quad (7)$$

So, for very large values of M , one has:

$$e^{-\beta\mathcal{H}} \simeq (e^{-\tau\mathcal{K}} e^{-\tau\mathcal{V}})^M \quad (8)$$

The density matrix of a system of N particles in the *primitive approximation* is given by the following path integral:

$$\rho(\mathbf{R}_0, \mathbf{R}_M; \beta) = (4\pi\lambda\tau)^{DNM/2} \int \dots \int d\mathbf{R}_1 \dots d\mathbf{R}_{M-1} \exp \left\{ \sum_{i=1}^M \left[\frac{(\mathbf{R}_{i-1} - \mathbf{R}_i)^2}{4\lambda\tau} + \frac{\tau}{2} (V(\mathbf{R}_{i-1}) + V(\mathbf{R}_i)) \right] \right\} \quad (9)$$

The system's partition function writes:

$$Z = \iint d\mathbf{R}_0 d\mathbf{R}_M \rho(\mathbf{R}_0, \mathbf{R}_M; \beta) \quad (10)$$

Note that this partition function is similar to the partition function of a classical system of N polymers. *Thus, evaluating the average value of any observable of the initial many-body quantum system is equivalent to evaluating the average value of the observable in the classical system described by the partition function Z given by eqs. (9), (10).*

So far we dealt with distinguishable particle wave functions. As we know the bosonic wave functions are symmetric and the fermionic ones are antisymmetric. This writes:

$$\Phi_{B/F}(\mathbf{R}) = (\pm)^{\mathcal{P}} \Phi_D(\mathcal{P}\mathbf{R}) \quad (11)$$

where the indexes B and F stand for bosonic / fermionic and \mathcal{P} is one of the $N!$ permutations between the particle labels of the N particle the many-body coordinate \mathcal{R} . The sign $+$ corresponds to bosonic systems and the sign $-$ to the fermionic ones. One can obtain the (anti)symmetrization by applying the (anti)symmetrization operators on the distinguishable particle wave-function:

$$\Phi_{B/F}(\mathbf{R}) = \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} (\pm)^{\mathcal{P}} \Phi_D(\mathcal{P}\mathbf{R}) \quad (12)$$

so,

$$\rho_{B/F}(\mathbf{R}, \mathbf{R}'; \beta) = \frac{1}{N!} \sum_{\mathcal{P}} (\pm)^{\mathcal{P}} \rho_D(\mathbf{R}, \mathcal{P}\mathbf{R}'; \beta) \quad (13)$$

and, replacing ρ_D with the corresponding path integral:

$$\rho_{B/F}(\mathbf{R}, \mathbf{R}'; \beta) = \frac{1}{N!} \sum_{\mathcal{P}} (\pm)^{\mathcal{P}} \int \dots \int d\mathbf{R}_1 \dots d\mathbf{R}_{M-1}$$

$$\rho_D(\mathbf{R}, \mathbf{R}_1; \beta) \dots \rho_D(\mathbf{R}_{M-1}, \mathcal{P}\mathbf{R}'; \beta) \quad (14)$$

Now, having the bosonic and fermionic partition functions of the polymer-like system we can readily perform Metropolis Monte Carlo simulations in order to estimate average values of various observables. The principle is to generate a trajectory in the system's configuration space in agreement with the detailed balanced principle. We will not insist here on the simulation since such methods are extensively explained elsewhere [13]. However, it is worth noticing that when sampling fermions we deal with both positive and negative statistical weights since the average value of any observable writes:

$$\langle O \rangle = \frac{\sum_{\mathcal{P}} (-1)^{\mathcal{P}} \int d\mathbf{R} d\mathbf{R}' \langle \mathbf{R} | O | \mathcal{P}\mathbf{R}' \rangle \rho(\mathbf{R}, \mathcal{P}\mathbf{R}'; \beta)}{\sum_{\mathcal{P}} (-1)^{\mathcal{P}} \int d\mathbf{R} d\mathbf{R}' \rho(\mathbf{R}, \mathcal{P}\mathbf{R}'; \beta)} \quad (15)$$

Therefore, we have the ratio between two differences. The problem arises at small temperatures where both differences are close to zero so that the statistical fluctuations increase dramatically. This effect is known as *the fermion sign problem*. However, since we perform simulations for highly excited nuclear-like systems the *fermion sign problem* shouldn't play here a big role.

Using the above exposed theoretical ingredients we perform Monte Carlo simulations for LJ bosonic and fermionic systems. The Lennard-Jones 6-12 (LJ) potential writes:

$$v_0(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (16)$$

We use the truncated and long-range corrected version of the above potential: $v(r) = v_0(r)$ when $r < r_c$; $v(r) = 0$ when $r \geq r_c$, corrections being subsequently included in order to account for the effect of the neglected tail [19]. We took $r_c = L/2$, L being the size of the recipient, $\sigma = 2.55$ fm and $\epsilon = 25.03$ MeV. These values are rather arbitrary but roughly describe the binding energies of various size nuclei. We simulated 16 quantum particles placed in a cubic recipient with periodic boundary conditions. Then, we construct the phase diagram of this system in both bosonic and fermionic quantics. To this aim, we estimate pressure versus volume curves at constant temperature. Pressure can be easily evaluated starting from its canonical definition: $P = T \partial \ln Z(\beta, V) / \partial V$, where $Z(\beta, V)$ is the system's canonical partition function as defined above. One gets the virial expression for pressure:

$$P = \frac{NT}{V} - \frac{1}{3V} \left\langle \sum_{i < j} r_{ij} \frac{\partial v(r_{ij})}{\partial r_{ij}} \right\rangle, \quad (17)$$

where $v(r_{ij})$ is the particle-particle interaction and $\langle \rangle$ has the meaning of canonical average.

Now let us discuss the results of the simulation. In Fig. 1 we represented pressure versus volume curves

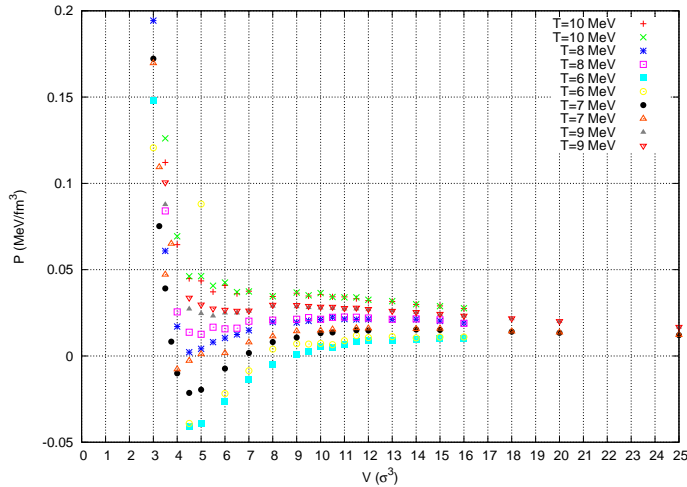


FIG. 1: Isothermal bosonic and fermionic pressure versus volume curves corresponding to various temperatures for a 16 particle system.

corresponding to both fermionic and bosonic 16 particle systems at temperatures ranging from 6 to 10 MeV. One can observe the backbendings of these curves, signatures of a first order liquid-gas phase transition. For a given temperature one can observe that all fermionic curves are above the bosonic ones. This can be better observed in Fig. 2 where bosonic and fermionic pressure versus volume curves corresponding to a temperature of 7 MeV are represented. One further performs Maxwell constructions on all collected pressure versus-volume curve and identify the liquid-gas coexistence region for both fermionic and bosonic systems. This result is illustrated in Fig. 3. There one can observe the phase diagrams of both fermionic and bosonic systems. Some interesting aspects are to be noticed: The fermionic coexistence region is wider than the bosonic one. The distance between the fermionic and the bosonic curves is larger on the denser branch of the phase diagram as expected since the quantum interaction between particles is supposed to be larger in that region. Finally, the critical point of both bosonic and fermionic systems appears to be the same, having the value of 10 MeV. This last point is particularly interesting showing that after the critical point the quantum effects are no longer important, after that region both systems having a gas-like behaviour. Taking into account the small size of the systems ($A=16$), the obtained critical point temperature, is *quite good*. In infinite nuclear systems the critical temperature is supposed to be higher, critical temperature being smaller as the size of the system decreases [7]. Indeed, from Ref. [7] one can deduce a ratio of about 1.58 between the critical temperature of an infinite system and the critical temperature of an $A=16$ system. One can therefore multiply the critical temperature found herein of 10 MeV with the factor 1.58 and deduce the critical temperature of an infinite system, $T = 15.8$ MeV which is a quite realistic

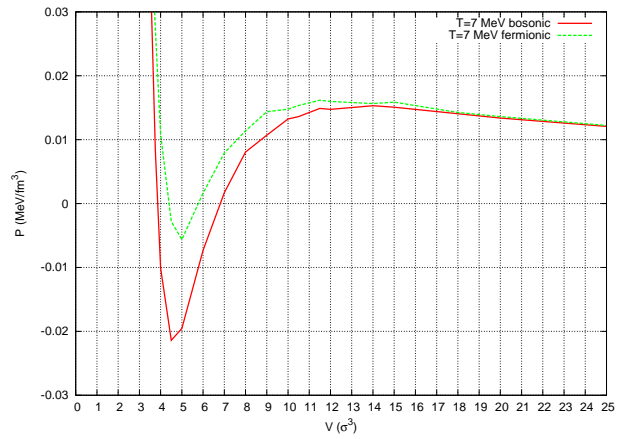


FIG. 2: Isothermal bosonic and fermionic pressure versus volume curves corresponding to a $T=7$ MeV temperature for a 16 particle system.

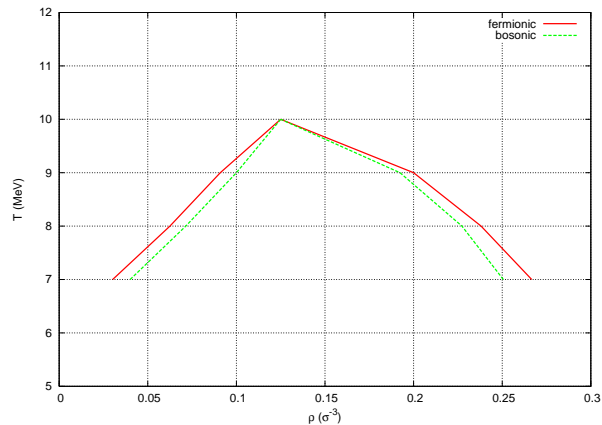


FIG. 3: Phase diagram of a bosonic and a fermionic 16 particle system in a box with PBC conditions.

value.

One can conclude that the Path Integral Monte Carlo is a powerful tool for investigating highly excited nuclear systems. Though the systems under consideration are rather small, still valuable information is obtained concerning the quantum effects on the systems' phase diagram. It was shown that both bosonic and fermionic have a common critical point. Moreover, the critical temperature value of 10 MeV obtained for an $A=16$ system appears to be realistic, leading via extrapolation to a value of 15.8 MeV for infinite systems.

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 $\Delta v = \frac{1}{2}\rho A \int_{r_c}^{\infty} \mathbf{dr} v(r) = 8\pi\rho A\epsilon[\sigma^{12}/(9r_c^9) - \sigma^6/(3r_c^3)];$
 $\Delta \mathcal{V} = \frac{1}{2}\rho A \int_{r_c}^{\infty} \mathbf{dr} (r \partial v(r)/\partial r) = 8\pi\rho A\epsilon[4\sigma^{12}/(9r_c^9) - 2\sigma^6/(3r_c^3)].$